

EXOTIC MOLECULES IN SPACE: A COORDINATED ASTRONOMICAL LABORATORY AND THEORETICAL STUDY

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Exotic Molecules in Space: A Coordinated Astronomical, Laboratory and Theoretical Study

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Annual Progress Report 3/31/01 through 3/31/02

The present report covers the second year of a grant which represents a direct continuation of NASA NAG5-4050, with the same title as before. It is dedicated as before to the discovery and characterization of new astrophysical molecules. The second year of this grant continues the rich vein of discoveries described in the previous year's report, with the publication or submission of the 11 papers listed below. Nearly all of these articles have appeared or will soon appear in leading refereed journals of astrophysics, chemical physics, and spectroscopy. Two are major invited reviews, one in *Spectrochimica Acta* (#1), the other in *Chemical Society Reviews* (#2).

The papers listed below describe the laboratory detection of 21 molecules of astrophysical interest, nearly all not previously observed, and nearly all of astrophysical interest as plausible candidates for the interstellar gas and circumstellar shells. The laboratory astrophysics of the whole set is complete, in the sense that the entire radio spectrum of each molecule is now determined to very high accuracy--of the order of one part in 10^7 . One of the most interesting of the new molecules is the organic ring $c\text{-C}_5\text{H}$ (#4 below), a molecule very similar to the most abundant organic ring in the interstellar gas, cyclopropenylidene $c\text{-C}_3\text{H}_2$, discovered previously by our group in both the laboratory and space. Efforts to find this fundamental new ring in space are underway, and we think stand a very good chance of success.

A major theme of our current research, described in detail in the final report of the last grant NAG5-4050, is the laboratory discovery of an optical molecular band exactly coinciding in frequency with the optical diffuse interstellar band (DIB) $\lambda 4430$, the strongest and most widely studied of the enigmatic interstellar spectral features which have been called the outstanding unsolved problem in astrophysical spectroscopy. In spite of much effort, we have not yet succeeded in fully determining the structure of the molecule responsible for the laboratory band, but, as discussed in the previous annual report, the evidence points to a fairly simple carbon ring or chain with the elemental formula C_nH_5 , where n , the

number of carbon atoms, is probably between 3 and 6, inclusive. Our laboratory work, done with a laser cavity ringdown spectrometer (CRDS) constructed over the past three years, may represent the most significant advance in DIB research in many years. A new laser spectrometer, one based on resonance enhanced multi-photon ionization (REMPI) with mass selection has been constructed in an attempt to determine exactly the carrier of laboratory $\lambda 4430$, and is now being tested on standard molecules. It will be used to shed further light on the carrier of $\lambda 4430$ in the fairly near future.

Our Fourier-transform microwave spectrometer, the instrument which has been responsible for the discovery of most of the nearly 100 new molecules discovered over the past four years in this laboratory, has been significantly improved during the present grant period. The instrument is now able to undertake extended spectral line surveys for periods of several days under computer control, while fully and stably cooled to the temperature of liquid nitrogen. By markedly reducing instrumental noise, cooling enhances the sensitivity of this already sensitive instrument by a factor of four, and has allowed the detection of molecules which could not have been found otherwise.

An accomplished spectroscopist from Spain, Maria Eugenia Sanz, of the University of Valladolid, is now in the second of a two year visit here. Dr. Sanz is largely supported by a postdoctoral grant from the Spanish government. Guido Fuchs, a graduate student in physics at the University of Cologne (Germany) under the supervision of Prof. Gisbert Winnewisser, visited for over three months during the past year and undertook three very productive investigations: (i) a systematic study of our nozzle discharge source; (ii) an exhaustive study of the hyperfine structure of the C_3N radical; and (iii) the discovery of the C_6N radical, an entirely new reactive molecule. Several articles describing this research are being prepared.

PUBLICATIONS UNDER NAG5-9379 IN 2001

1. "Carbon Chains and Rings in the Laboratory and in Space," P. Thaddeus and M. C. McCarthy, 2001, *Spectrochimica Acta*, **A 57**, 757-774.
2. "Microwave and Laser Spectroscopy of Carbon Chains and Rings," Michael C. McCarthy and Patrick Thaddeus, 2001, *Chemical Society Reviews*, **30**, 177-185.
3. "Rotational Spectra of Sulfur Carbon Chains: I The Radicals C_4S , C_5S , C_6S , C_7S , C_8S , and C_9S ," V. D. Gordon, M. C. McCarthy, A. J. Apponi, and P. Thaddeus, 2001, *Astrophysical Journal Supplement*, **134**, 311.
4. "The Cyclic C_5H Radical," A. J. Apponi, M. E. Sanz, C. A. Gottlieb, M. C. McCarthy, and P. Thaddeus, 2001, *Astrophysical Journal Letters*, **547**, L65.
5. "Rotational Spectra of Sulfur Carbon Chains II: HC_5S , HC_6S , HC_7S , & HC_8S , and H_2C_4S , H_2C_5S , H_2C_6S , & H_2C_7S ," V. D. Gordon, M. C. McCarthy, A. J. Apponi, and P. Thaddeus, 2001, *Astrophysical Journal Supplement*, in press.
6. "Rotational Spectra of $SiCN$, $SiNC$, and the SiC_nH ($n = 2, 4-6$) Radicals," M. C. McCarthy, A. J. Apponi, C. A. Gottlieb, and P. Thaddeus, 2001, *Journal of Chemical Physics*, **115**, 870.
7. "EGRET Observations of Monoceros: Diffuse Gamma-Ray Emission in the Outer Galaxy," S. W. Digel, I. A. Grenier, S. D. Hunter, T. M. Dame, and P. Thaddeus, 2001, *Astrophysical Journal*, **555**, 12.
8. "The Rotational Spectra of H_2CCSi and H_2C_4Si ," M. C. McCarthy and P. Thaddeus, 2001, *Journal of Molecular Spectroscopy*, in press.
9. "Carbon-13 Isotopic Species of H_2C_3 , H_2C_4 , and H_2C_5 : High-Resolution Rotational Spectra," M. C. McCarthy and P. Thaddeus, 2001, *Journal of Molecular Spectroscopy*, in press.
10. "Laboratory Detection of a Bent-Chain Carbene Isomer of C_6H_2 ," M. C. McCarthy and P. Thaddeus, 2001, *Astrophysical Journal Letters*, submitted.
11. "Ab Initio Theory and Rotational Spectra of Linear Carbon Chains SiC_nS ," Peter Botschwina, M. Eugenia Sanz, Michael C. McCarthy, and P. Thaddeus, 2001, *Journal of Chemical Physics*, submitted.